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COLLISIONS OF POLARIZED ELECTRONS WITH O_2

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ABSTRACT

Recently several methods have been developed and applied to studies of electron-molecule collisions at low impact energies. These approaches include the R-matrix, Linear algebraic, complex Kohn, and Schwinger multichannel (SMC) methods. In principle, these methods can account for important physical effects in such collisions which arise from open and closed electronic channels. In this paper we will report some results of preliminary studies of collisions of low-energy electrons with molecular oxygen, an open-shell system. In contrast to closed-shell systems such as H_2 and N_2, the electron polarization may change in collisions with these open-shell targets due to spin-exchange processes. We have determined these spin-exchange effects for elastic e-O_2 collisions and found them to be much smaller than those seen in alkali atoms such as Na. Our results compare well with those of recent measurements of these effects for O_2 by Hanne and his collaborators.

BACKGROUND AND RESULTS

In recent years there has been significant progress in theoretical studies of electron-molecule collision processes. Several ab-initio methods are now available for carrying out studies of elastic and inelastic electron-molecule collisions. These include the R-matrix,[1] the Linear algebraic,[2] the Schwinger Multichannel (SMC),[3] and the complex Kohn methods.[4] In principle, these methods can account for important physical effects in such collisions which arise from closed and open channels. In some cases, recent advances in computer technology also now allow these methods to be applied to large molecular systems where such studies would have been previously impractical.[5]

In this paper we will discuss some preliminary results of an extension and application of the SMC method to electron collisions with open-shell molecules. An important goal of this effort has been to examine elastic scattering of polarized electrons by O_2. To date the vast majority of theoretical and experimental studies have been with unpolarized electron beams and randomly oriented molecules. There has also been no spin analysis of the scattered electron. There have been some studies of unpolarized electron scattering by an oriented molecule.[6] The lack of spin selection yields a cross section which is averaged over several spin configurations and in which the underlying dynamics of these processes is masked. Experiments with electron-photon coincidence[7] and on superelastic scattering of electrons by laser-excited systems[8] provide significant additional information on the dynamics of these collisions. Although most such studies have been on atoms where suitable theoretical methods are available,[9] there have been few applications to molecular systems.[10] Experiments with polarized electron beams can provide even further dynamical insight into these collisions.[11] Currently available spin-polarized sources with the same currents as unpolarized sources,[12] coupled with spin analysis of the scattered beam, now make possible experiments which provide even more detailed information about these collision processes.[13]

We chose the O_2 molecule as a starting point because in open-shell molecules, spin-flip effects already appear in the elastic channel. Moreover, spin exchange cross sections for elastic scattering of polarized electrons from O_2 have already been measured at thermal energies.[14] The ground state of an open-shell molecule has a total electronic spin S_i different from zero. Electron scattering by this molecule hence has two spin-irreducible scattering amplitudes corresponding each to a total spin (electron+molecule) $S = S_i \pm 1/2$. The presence of two different scattering amplitudes allows the spin-flip exchange process to occur. In simple terms, an electron can be elastically scattered by an open-shell molecule but leave it in a different magnetic sub-level M_{S_i}. Earlier studies of electron collisions with O_2 have been concerned with excitation processes.[15,16]

Our scattering calculation included the ${}^3\Sigma_g^-$ ground state of O_2 and the ${}^1\Delta_g$ and ${}^1\Sigma_g^+$ excited states. These states all arise from the ground state electron configuration. This is, hence, a three-state calculation of O_2. We have used a Hartree-Fock description for the O_2 molecule, whose ground state electron configuration is given by $(1\sigma_g)^2\ (1\sigma_u)^2\ (2\sigma_g)^2\ (2\sigma_u)^2\ (3\sigma_g)^2\ (1\pi_u)^4\ (1\pi_g)^2$.

The elastic differential cross section for unpolarized electron scattering is given by:

$$\frac{d\sigma}{d\Omega} = \frac{2}{3} \mid f^{(\frac{3}{2})} \mid^2 + \frac{1}{3} \mid f^{(\frac{1}{2})} \mid^2$$

where $f^{(S)}$ is the scattering amplitude with total spin S. Our calculated differential cross sections for elastic scattering of unpolarized electrons by O_2 at energies of 5ev, 10ev, and 20ev are in good agreement with the experimental results of Trajmar et al.[17]

The spin-flip differential cross section is given by:

$$\frac{d\sigma_{sf}}{d\Omega} = \frac{4}{27} \mid f^{(\frac{3}{2})} - f^{(\frac{1}{2})} \mid^2 \quad ,$$

showing that spin-flip processes arise from the difference between $f^{(\frac{3}{2})}$ and $f^{(\frac{1}{2})}$. These amplitudes $f^{(\frac{3}{2})}$ and $f^{(\frac{1}{2})}$ reflect the dynamics of the interaction of the continuum electron and the molecule. But it is the exchange interaction between the scattered electron and target electrons that affects $f^{(\frac{3}{2})}$ and $f^{(\frac{1}{2})}$ asymmetrically. As a result the spin-flip cross section gives information about the exchange interaction in these collisions. Our calculated results compare well with recent measurements of Hanne and collaborators[18] of the electron polarization before and after collisions with O_2 at 5ev and 10ev.

Measurements of spin exchange at thermal energies[14] and beam studies with polarized electrons[18] both indicate that electron exchange in collisions with O_2 is substantially smaller than with alkali-metal atoms. Our calculated results support these observations. Our spin-flip cross section for elastic e-O_2 scattering is of the same order of magnitude as the excitation cross section for the $^1\Delta_g$ and $^1\Sigma_g^+$ states. These are also pure exchange excitation processes. The significant question now becomes: why do alkali-metal atoms have such a large spin-flip cross section? We will show that this is related to resonances, interferences, and geometrical effects which will be discussed in a future publication.[19]

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